

10/S82,609

10/513699

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAEAL1624

PASSWORD:917P742

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *

SESSION RESUMED IN FILE 'CASREACT' AT 18:01:31 ON 13 AUG 2007

FILE 'CASREACT' ENTERED AT 18:01:31 ON 13 AUG 2007

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ENTER STRUCTURE FORMAT (SIM), NOS:ide

'IDE' IS NOT A VALID STRUCTURE FORMAT KEYWORD

Structure Formats

SIA ----- Structure Image, Attributes, and map table if it contains data. (Default)

SIM ----- Structure IMage.

SAT ----- Structure ATtributes and map table if it contains data.

SCT ----- Structure Connection Table and map table if it contains data.

SDA ----- All Structure DAta (image, attributes, connection table and map table if it contains data).

NOS ----- NO Structure data.

ENTER STRUCTURE FORMAT (SIM), NOS:end

=> .

. IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.

For a list of commands available to you in the current file, enter

"HELP COMMANDS" at an arrow prompt (>).

=> file casreact

COST IN U.S. DOLLARS

SINCE FILE

ENTRY

TOTAL

FULL ESTIMATED COST

SESSION

234.75 938.13

FILE 'CASREACT' ENTERED AT 18:05:20 ON 13 AUG 2007

USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

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FILE CONTENT:1840 - 11 Aug 2007 VOL 147 ISS 8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

*

* CASREACT now has more than 12 million reactions

*

*

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EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	501	(546/121,546/83,544/333,544/127). CCLS.	US-PGPUB; USPAT	OR	OFF	2007/08/13 17:19
L2	1	L1 AND DIHYDROPYRANO	US-PGPUB; USPAT	OR	ON	2007/08/13 17:20
L3	1	L2 AND IMIDAZO	US-PGPUB; USPAT	OR	ON	2007/08/13 17:20
L4	1	L3 AND PYRIDINE	US-PGPUB; USPAT	OR	ON	2007/08/13 17:20

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Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>

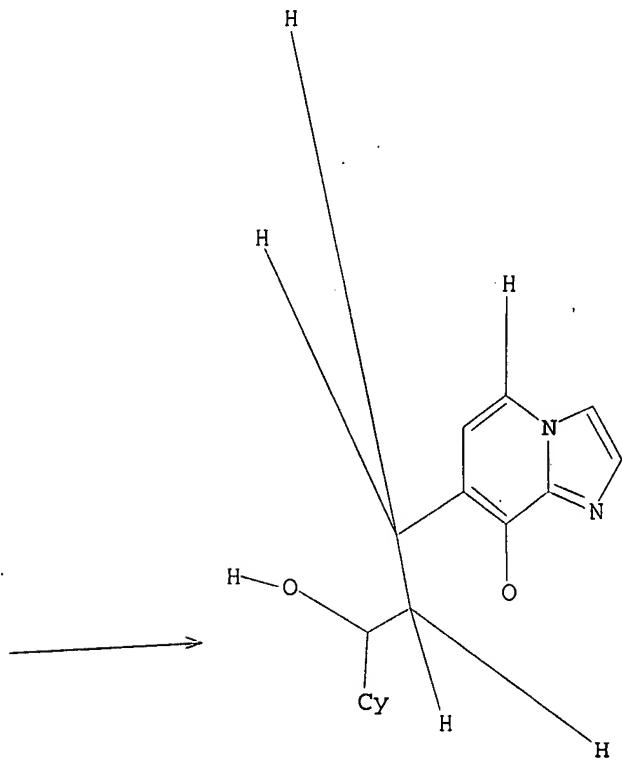
Uploading C:\Program Files\Stnexp\Queries\10582609b.str

L17 STRUCTURE UPLOADED

=> d 117

L17 HAS NO ANSWERS

L17 STR



Structure attributes must be viewed using STN Express query preparation.

=>

Uploading C:\Program Files\Stnexp\Queries\10582609a.str

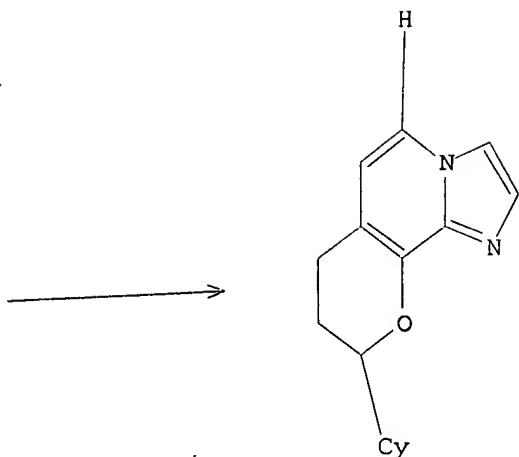
L18 STRUCTURE UPLOADED

=> d 118

L18 HAS NO ANSWERS

L18 STR

10/513699



Structure attributes must be viewed using STN Express query preparation.

=> s l17 full

FULL SEARCH INITIATED 18:06:08 FILE 'CASREACT'

SCREENING COMPLETE - 46 REACTIONS TO VERIFY FROM

6 DOCUMENTS

100.0% DONE 46 VERIFIED 0 HIT RXNS
SEARCH TIME: 00.00.01

0 DOCS

L19 0 SEA SSS FUL L17 (0 REACTIONS)

=> s l18 full

FULL SEARCH INITIATED 18:06:13 FILE 'CASREACT'

SCREENING COMPLETE - 1191 REACTIONS TO VERIFY FROM

57 DOCUMENTS

100.0% DONE 1191 VERIFIED 10 HIT RXNS
SEARCH TIME: 00.00.01

2 DOCS

L20 2 SEA SSS FUL L18 (10 REACTIONS)

=> d ibib abs fhit

L20 ANSWER 1 OF 2 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 111:77237 CASREACT

TITLE: Antiulcer agents. 4. Conformational considerations and the antiulcer activity of substituted imidazo[1,2-a]pyridines and related analogs

AUTHOR(S): Kaminski, James J.; Puchalski, Chester; Solomon, Daniel M.; Rizvi, Razia K.; Conn, David J.; Elliott, Arthur J.; Lovey, Raymond G.; Guzik, Henry; Chiu, P. J. S.; et al.

CORPORATE SOURCE: Pharm. Res. Div., Schering Res., Bloomfield, NJ, 07003, USA

SOURCE: Journal of Medicinal Chemistry (1989), 32(8), 1686-700
CODEN: JMCMAR; ISSN: 0022-2623

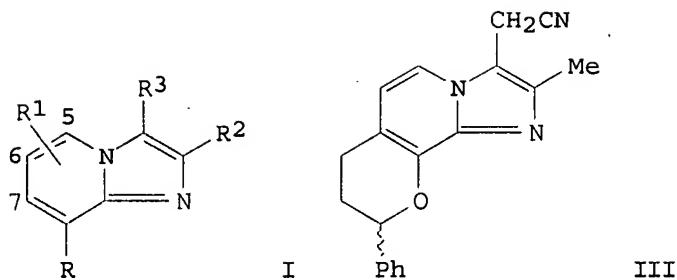
DOCUMENT TYPE: Journal

LANGUAGE: English

GI

<12/04/2007>

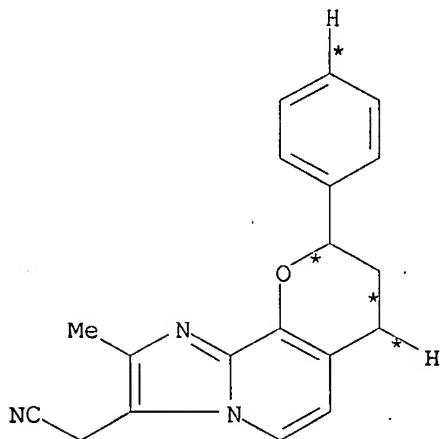
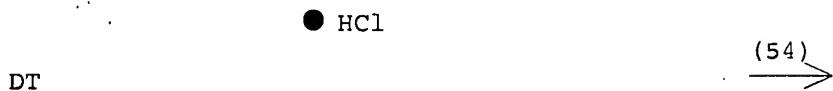
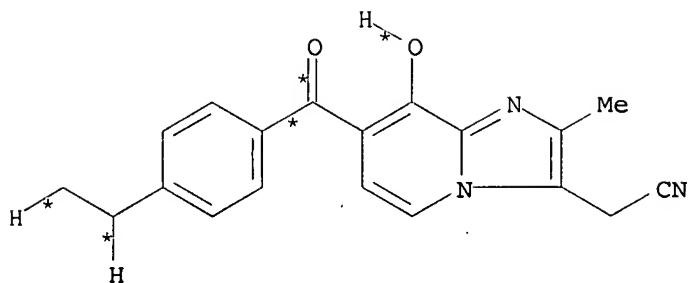
Erich Leese



AB Definition of the interrelationship between the conformational characteristics of a series of substituted imidazo[1,2-a]pyridines and their antiulcer activity was investigated by examining the conformational properties of imidazo[1,2-a]pyridine I [R = PhCH₂O, R₁ = H, R₂ = Me, R₃ = CH₂CN (II)], by using a variety of exptl. and theor. methods. The result of these studies was the identification of two distinctly different candidates, designated the folded and the extended conformation, resp., to represent the two possible min.-energy conformations of II. In order to select the biol. relevant conformer, a group of 3-substituted 2-methylimidazo[1,2-a]pyridines, having either a cis- or a trans-2-phenylethenyl substituent at the 8-position, were designed as conceptually simple and synthetically accessible semirigid analogs of the resp. candidate conformers. Gastric antisecretory activity was found to reside only in the trans isomers I (R = trans-PhCH:CH, R₁ = H, R₂ = Me; R₃ = Me, CH₂CN, NH₂), which mimic the extended conformation. This observation led to the construction of imidazo[1,2-a]pyrano[2,3-c]pyridine-3-acetonitrile (III), a rigid tricyclic analog that is effectively locked in the extended conformation and that exhibited an antiulcer profile comparable to that of prototype II. These results unequivocally demonstrate that, in accord with expectation for a drug operating at a specific receptor, the conformational characteristics of the mol. have a substantial effect in determining its antiulcer activity. More precisely, it has been demonstrated that it is the extended conformation of II that represents the bioactive form of the drug. These results constitute the basis for a mol. probe that should aid in the investigation of the as yet uncharacterized gastric proton pump enzyme (H⁺/K⁺-ATPase), by means of which II and its analogs presumably exert their pharmacol. actions.

RX(54) OF 213 . . . DT ==> DU . . .

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DU

RX(54) RCT DT 121394-50-1

STAGE(1)

RGT C 16940-66-2 NaBH4
SOL 64-17-5 EtOH, 75-09-2 CH₂Cl₂

STAGE(2)

RGT DV 109-63-7 BF₃-Et₂O
SOL 75-09-2 CH₂Cl₂

PRO DU 93749-57-6

NTE sand used in second step

=> d ibib abs hitstr 2
'HITSTR' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS ----- GI and AB
ALL ----- BIB, AB, IND, RE, Single-step Reactions
APPS ----- AI, PRAI
BIB ----- AN, plus Bibliographic Data
CAN ----- List of CA abstract numbers without answer numbers
CBIB ----- AN, plus Compressed Bibliographic Data
DALL ----- ALL, delimited (end of each field identified)
IABS ----- ABS, indented with text labels
IALL ----- ALL, indented with text labels
IBIB ----- BIB, indented with text labels
IND ----- Indexing data
IPC ----- International Patent Classifications
ISTD ----- STD, indented with text labels
OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations

MAX ----- Same as ALL
PATS ----- PI, SO
SCAN ----- TI and FCRD (random display, no answer number. SCAN must be entered on the same line as DISPLAY, e.g., D SCAN.)
SSRX ----- Single-Step Reactions (Map, Diagram, and Summary for all single-step reactions)
STD ----- BIB, IPC, and NCL

CRD ----- Compact Display of All Hit Reactions
CRDREF ----- Compact Reaction Display and SO, PY for Reference
FHIT ----- Reaction Map, Diagram, and Summary for first hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ----- First hit in Compact Reaction Display (CRD) format
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with CA reference information (SO, PY). (Default)
FPATH ----- PATH, plus Reaction Summary for the "long path"
FSPATH ----- SPATH, plus Reaction Summary for the "short path"
HIT ----- Reaction Map, Reaction Diagram, and Reaction Summary for all hit reactions and fields containing hit terms
OCC ----- All hit fields and the number of occurrences of the hit terms in each field. Includes total number of HIT, PATH, SPATH reactions. Labels reactions that have incomplete verifications.
PATH ----- Reaction Map and Reaction Diagram for the "long path". Displays all hit reactions, except those whose steps are totally included within another hit reaction which is displayed
RX ----- Hit Reactions (Map, Diagram, Summary for all hit reactions)
RXG ----- Hit Reaction Graphics (Map and Diagram for all hit reactions)
RXL ----- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS ----- Hit Reaction Summariers (Map and Summary for all hit reactions)
SPATH ----- Reaction Map and Reaction Diagram for the "short path". Displays all single step reactions which contain a hit substance. Also displays those multistep reactions that have a hit substance in both the first and last steps of the reaction, except for

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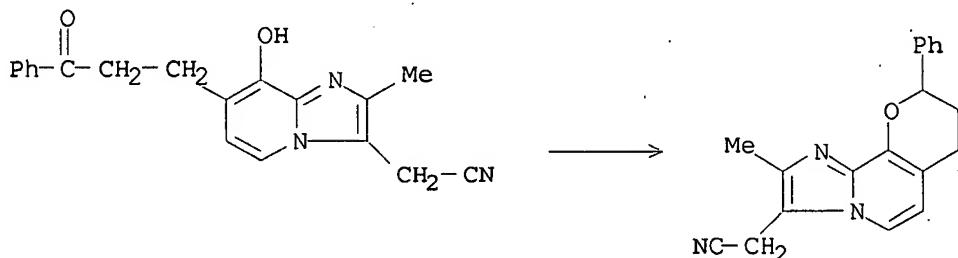
those hit reactions whose steps are totally included within another hit reaction which is displayed

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (>). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

ENTER DISPLAY FORMAT (FCRDREF) : .

L20 ANSWER 2 OF 2 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 3



REF: U.S., 4468400, 28 Aug 1984

=> d his

(FILE 'HOME' ENTERED AT 17:27:32 ON 13 AUG 2007)

FILE 'REGISTRY' ENTERED AT 17:27:41 ON 13 AUG 2007

L1 STRUCTURE uploaded
L2 189 S L1 FULL

FILE 'CAPLUS' ENTERED AT 17:28:17 ON 13 AUG 2007
L3 25 S L2 FULL

FILE 'REGISTRY' ENTERED AT 17:30:26 ON 13 AUG 2007
L4 STRUCTURE uploaded
L5 189 S L1 FULL
L6 20 S L4 FULL
L7 11 S L1
L8 1 S L4

FILE 'REGISTRY' ENTERED AT 17:42:10 ON 13 AUG 2007
L9 STRUCTURE uploaded
L10 189 S L9 FULL

FILE 'CAPLUS' ENTERED AT 17:42:34 ON 13 AUG 2007
L11 25 S L10 FULL

FILE 'CASREACT' ENTERED AT 17:46:49 ON 13 AUG 2007

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L12 STRUCTURE UPLOADED
L13 STRUCTURE UPLOADED
L14 0 S L12
L15 2 S L12 FULL
L16 0 S L13 FULL

FILE 'CASREACT' ENTERED AT 18:05:20 ON 13 AUG 2007

L17 STRUCTURE UPLOADED
L18 STRUCTURE UPLOADED
L19 0 S L17 FULL
L20 2 S L18 FULL